frontiers

Supplementary Material

ANO1-Downregulation Induced by Schisandrathera D: A Novel Therapeutic Target for the Treatment of Prostate and Oral Cancers

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Supplementary Table S1: Interaction analysis of ANO1 with Schisandrathera D and Ani9

Compound name (Docked with ANO1)	Hydrogen bonds (Distance in Å)	Hydrophobic interactions (Distance in Å)	π stacking	Halogen bond
Schisandrathera D-ANO1 (PDB ID: 5OYB)	His^{650} (1.84)	Ala^{697} (3.85)		Asn^{647} (3.70)
	His^{661} (1.79)	Pro^{701} (3.32)		
		Pro^{701} (3.53)		
	His^{695} (1.82)	Lys^{741} (3.59)		
		Leu^{746} (3.90)		
Schisandrathera D-ANO1 (PDB ID: 6BGJ)	Asn^{647} (3.02)	Glu^{701} (3.58)		
	Glu^{701} (1.99)			
	Lys^{737} (2.13)			
Ani9-ANO1 (PDB ID: 5OYB)		Leu^{699} (3.71)	Lys^{327} (4.41)	
			Lys^{574} (3.97)	
Ani9-ANO1 (PDB ID: 6BGJ)		Leu^{543} (3.97)		
		Leu^{639} (3.73)		
		Leu^{643} (3.50)		
		Glu^{701} (3.80)		
		Ile^{704} (3.52)		

Supplementary Table S2: Molecular docking and molecular mechanics – generalized Born surface area scores

ANO1 PDB ID	Docking score		MM-GBSA score	
	5OYB	6BGJ	5OYB	6BGJ
Schisandrathera D	–5.042	–5.589	–29.10	–41.78
Ani9	–4.095	–4.612	–33.08	–29.10

*Energy unit is kcal·mol^{-1}.
Legend: PDB, Protein Data Bank; MM-GBSA, molecular mechanics – generalized Born surface area